Neural Navier-Stokes equations

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1 Formulation

1.1 Reynolds averaged Navier-Stokes equations

Consider a wind velocity field, denoted by $\boldsymbol{u} = [u_x, u_y, u_z]^T$, that obeys the Navier-Stokes equations

$$\partial_t \boldsymbol{u} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = -\rho^{-1}\nabla p + \nu \nabla^2 \boldsymbol{u}, \tag{1}$$

$$\nabla \cdot \boldsymbol{u} = 0, \tag{2}$$

where density ρ is assumed to be constant, p is the fluid pressure, and ν is the kinematic viscosity. The forcing terms arising from gravity, Coriolis force, etc. are neglected. The ground is located at the plane $z = 0$, where the velocity vanishes.

We consider a decomposition of the instantaneous flow characteristics, i.e. the velocity $\boldsymbol{u}$ and the pressure p, into a base flow $(\boldsymbol{U}, P)$, turbulent fluctuations $(\boldsymbol{u}', p')$, and a perturbed flow $(\tilde{\boldsymbol{u}}, \tilde{p})$

$$\boldsymbol{u} = \boldsymbol{U} + \boldsymbol{u}' + \tilde{\boldsymbol{u}}, \quad p = P + p' + \tilde{p}, \tag{3}$$

where, denoting by overbar the time averaging, the perturbed flow given by

$$\tilde{\boldsymbol{u}} = \overline{\boldsymbol{u} - \boldsymbol{U}} = \overline{\boldsymbol{u}} - \boldsymbol{U}, \quad \tilde{p} = \overline{p - P} = \overline{p} - P, \tag{4}$$

is assumed to satisfy the following relation

$$\iint \tilde{\boldsymbol{u}} \, \mathrm{d}x\mathrm{d}y = 0. \tag{5}$$

In atmospheric boundary layers, the base flow $\boldsymbol{U} = [U_x(z), U_y(z), 0]^T$ with

$$U_x(z) = U\cos(\varphi)\frac{\ln(z/z_0 + 1)}{\ln(Z/z_0 + 1)}, \quad U_y(z) = U\sin(\varphi)\frac{\ln(z/z_0 + 1)}{\ln(Z/z_0 + 1)}, \tag{6}$$

is so selected that it vanishes on the ground and approaches the geostrophic wind speed at city's canopy $z = Z$. Here, the magnitude U and the orientation φ of the geostrophic wind measured at height Z are assumed known. The roughness length z_0 is a corrective measure accounting for the cumulative effect of the buildings. For urban areas, we take $z_0 = 1$ constant.

Substituting the decomposition (3) into the Navier-Stokes equations, the governing equations for the perturbed flow can be expressed in Einstein notation as

$$U_j \frac{\partial \tilde{u}_i}{\partial x_j} + \tilde{u}_z \frac{\partial U_i}{\partial z} + \tilde{b}_i = -\rho^{-1} \frac{\partial \overline{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left[\nu \left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i} \right) - \overline{u_i' u_j'} \right], \tag{7}$$

$$\frac{\partial \tilde{u}_i}{\partial x_i} = 0, \tag{8}$$

where the integration in time removes the temporal dependence and

$$b_i = \tilde{u}_j \frac{\partial \tilde{u}_i}{\partial x_j} \tag{9}$$

denotes the inertial term. The terms within the square bracket are the viscous stress due to molecular transfer and an additional Reynolds stress arising from turbulent fluctuations. In other words, turbulent fluctuations influence the progress of the mean flow in the way that the latter exhibits an apparent increase in resistance against deformation. To close the system of equations, we use the turbulent-viscosity hypothesis, which states that the deviatoric Reynolds stress is proportional to the mean rate of strain, cf. Chapter 4 in [1]

$$-\overline{u_i' u_j'} + \frac{1}{3} \delta_{ij} \overline{u_i' u_i'} = \nu_t \left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i} \right), \tag{10}$$

where $\nu_t = \nu_t(x, y, z)$ is the eddy viscosity and δ_{ij} is the Kronecker delta. With the logarithmic base flow (6), to the leading order, the eddy viscosity assumes a linear dependence on the vertical coordinate (cf. Chapter 11 in [2])

$$\nu_t(z) = \frac{u_\tau^2}{\partial_z \sqrt{U_x^2 + U_y^2}} = \frac{\kappa^2 U (z + z_0)}{\ln(Z/z_0 + 1)}, \tag{11}$$

where $u_\tau = \kappa U / \ln(Z/z_0 + 1)$ denotes the shear velocity and $\kappa = 0.41$ is the von Karman constant.

Substituting Eq. (10) into the mean momentum equation (7) gives

$$U_j \frac{\partial \tilde{u}_i}{\partial x_j} + \tilde{u}_z \frac{\partial U_i}{\partial z} + b_i = -\rho^{-1} \frac{\partial \overline{p}_\Sigma}{\partial x_i} + \nu_\Sigma \frac{\partial^2 \tilde{u}_i}{\partial x_j^2} + \frac{\partial \nu_\Sigma}{\partial z} \left(\frac{\partial \tilde{u}_z}{\partial x_i} + \frac{\partial \tilde{u}_i}{\partial z} \right) + \frac{\partial}{\partial z} \left(\nu_\Sigma \frac{\partial U_i}{\partial z} \right). \tag{12}$$

where the presence of turbulence augments the mean pressure field with turbulent kinetic energy and augments the molecular kinematic viscosity with eddy viscosity

$$\overline{p}_\Sigma = \overline{p} + \frac{1}{3} \rho \overline{u_i' u_i'} \quad \text{and} \quad \nu_\Sigma(x, y, z) = \nu + \nu_t(x, y, z). \tag{13}$$

Let us express Eqs. (12) componentwise

$$U_x \frac{\partial \tilde{u}_x}{\partial x} + U_y \frac{\partial \tilde{u}_x}{\partial y} + \tilde{u}_z \frac{\partial U_x}{\partial z} + \tilde{b}_x = -\rho^{-1} \frac{\partial \overline{p}_\Sigma}{\partial x} + \nu_\Sigma \nabla^2 \tilde{u}_x + \frac{\partial \nu_\Sigma}{\partial z} \left(\frac{\partial \tilde{u}_z}{\partial x} + \frac{\partial \tilde{u}_x}{\partial z} \right) + \frac{\partial}{\partial z} \left(\nu_\Sigma \frac{\partial U_x}{\partial z} \right), \tag{14a}$$

$$U_x \frac{\partial \tilde{u}_y}{\partial x} + U_y \frac{\partial \tilde{u}_y}{\partial y} + \tilde{u}_z \frac{\partial U_y}{\partial z} + \tilde{b}_y = -\rho^{-1} \frac{\partial \overline{p}_\Sigma}{\partial y} + \nu_\Sigma \nabla^2 \tilde{u}_y + \frac{\partial \nu_\Sigma}{\partial z} \left(\frac{\partial \tilde{u}_z}{\partial y} + \frac{\partial \tilde{u}_y}{\partial z} \right) + \frac{\partial}{\partial z} \left(\nu_\Sigma \frac{\partial U_y}{\partial z} \right), \tag{14b}$$

$$U_x \frac{\partial \tilde{u}_z}{\partial x} + U_y \frac{\partial \tilde{u}_z}{\partial y} + \tilde{b}_z = -\rho^{-1} \frac{\partial \overline{p}_\Sigma}{\partial z} + \nu_\Sigma \nabla^2 \tilde{u}_z + \frac{\partial \nu_\Sigma}{\partial z} \left(\frac{\partial \tilde{u}_z}{\partial z} + \frac{\partial \tilde{u}_z}{\partial z} \right). \tag{14c}$$

The preceding expression can be greatly simplified by taking the curl of the momentum equations in horizontal directions, leading to the velocity-vorticity formulation

$$\nu_\Sigma \nabla^2 \tilde{u}_z + 2 \frac{\partial \nu_\Sigma}{\partial z} \frac{\partial \tilde{u}_z}{\partial z} - U_x \frac{\partial \tilde{u}_z}{\partial x} - U_y \frac{\partial \tilde{u}_z}{\partial y} = \hat{\boldsymbol{z}} \cdot \tilde{\boldsymbol{b}} + \rho^{-1} \frac{\partial \overline{p}_\Sigma}{\partial z}, \tag{15}$$

$$\nu_\Sigma \nabla^2 \tilde{\omega}_z + \frac{\partial \nu_\Sigma}{\partial z} \frac{\partial \tilde{\omega}_z}{\partial z} - U_x \frac{\partial \tilde{\omega}_z}{\partial x} - U_y \frac{\partial \tilde{\omega}_z}{\partial y} = \hat{\boldsymbol{z}} \cdot \nabla \times \tilde{\boldsymbol{b}} + \frac{\partial U_y}{\partial z} \frac{\partial \tilde{u}_z}{\partial x} - \frac{\partial U_x}{\partial z} \frac{\partial \tilde{u}_z}{\partial y}. \tag{16}$$

The difficulty with the velocity-vorticity formulation is that the pressure and the inertial term $\tilde{\boldsymbol{b}}$ depend also on $\tilde{u}_x, \tilde{u}_y$; whereas the recovery of $\tilde{u}_x, \tilde{u}_y$ from $\tilde{u}_z$ and $\tilde{\omega}_z$ is not straightforward. Moreover, to determine the pressure term, the continuity equation must be evoked.

Note.

1. Consider a change of variables

$$x_L = x - \frac{U_x(z)}{U_y(z)} y, \quad y_L = y - \frac{U_y(z)}{U_x(z)} x, \tag{17}$$

the partial derivatives

$$\frac{\partial}{\partial x} = \frac{\partial x_L}{\partial x} \frac{\partial}{\partial x_L} + \frac{\partial y_L}{\partial x} \frac{\partial}{\partial y_L} = \frac{\partial}{\partial x_L} - \frac{U_y(z)}{U_x(z)} \frac{\partial}{\partial y_L}, \tag{18}$$

$$\frac{\partial}{\partial y} = \frac{\partial y_L}{\partial y} \frac{\partial}{\partial y_L} + \frac{\partial x_L}{\partial y} \frac{\partial}{\partial x_L} = \frac{\partial}{\partial y_L} - \frac{U_x(z)}{U_y(z)} \frac{\partial}{\partial x_L}, \tag{19}$$

such that

$$U_x(z) \frac{\partial}{\partial x} + U_y(z) \frac{\partial}{\partial y} = 0, \tag{20}$$

provided that $U_x(z) \neq 0$ and $U_y(z) \neq 0$.

2. At this level, assumption is made on the base flow $\boldsymbol{U}(z)$ and on the eddy viscosity ν_t.

1.2 Scale separation in atmospheric boundary layer

In the atmospheric boundary layer, the separation of characteristic length scales between the horizontal and vertical directions, denoted respectively by L and h, justifies scaling the horizontal directions by L while scaling the vertical direction by h

$$x = Lx^*, \quad y = Ly^*, \quad z = hz^*, \quad \eta = h/L \ll 1, \tag{21}$$

where the star denotes dimensionless variables. Substituting Eqs. (21) into the continuity equation reveals the following scaling relations for the velocities and for the vorticity

$$U_x = UU_x^*, \quad U_y = UU_y^*, \quad \tilde{u}_x = U\tilde{u}_x^*, \quad \tilde{u}_y = U\tilde{u}_y^*, \quad \tilde{u}_z = \eta U\tilde{u}_z^*, \quad \tilde{\omega}_z = (U/L)\tilde{\omega}_z^*. \tag{22}$$

The scaling for pressure

$$\overline{p}_\Sigma = \rho U^2 \overline{p}_\Sigma^*, \tag{23}$$

is so selected that the pressure gradient balances the inertia terms in the horizontal directions. Substituting Eqs. (21, 22, 23) into Eqs. (15) gives

$$Re_\eta^{-1}\left[\eta^2\partial_{x^*}^2 + \eta^2\partial_{y^*}^2 + \partial_{z^*}^2 + 2\left(\partial_{z^*}Re_\eta^{-1}\right)\partial_{z^*} - U_x^*\partial_{x^*} - U_y^*\partial_{y^*}\right]\tilde{u}_z^* = \hat{\boldsymbol{z}}\cdot\tilde{\boldsymbol{b}}^* + \eta^{-2}\partial_{z^*}\overline{p}_\Sigma^*, \tag{24a}$$

$$\begin{aligned} Re_\eta^{-1}\left[\eta^2\partial_{x^*}^2 + \eta^2\partial_{y^*}^2 + \partial_{z^*}^2 + \left(\partial_{z^*}Re_\eta^{-1}\right)\partial_{z^*} - U_x^*\partial_{x^*} - U_y^*\partial_{y^*}\right]\tilde{\omega}_z^* &= \hat{\boldsymbol{z}}\cdot\nabla\times\tilde{\boldsymbol{b}}^* \\ &+ \left(\partial_{z^*}U_y^*\right)\partial_{x^*}\tilde{u}_z^* - \left(\partial_{z^*}U_x^*\right)\partial_{y^*}\tilde{u}_z^*, \end{aligned} \tag{24b}$$

where $Re_\eta = \eta Uh/\nu_\Sigma$. In Eq. (24a), the vertical pressure gradient is too large to be balanced by prevailing inertial and viscous forces in the equation, hence it must be zero. Collecting terms of order $O(1)$, the mean momentum equations for boundary layers assume the form

$$Re_\eta^{-1}\left[\partial_{z^*}^2 + 2\left(\partial_{z^*}Re_\eta^{-1}\right)\partial_{z^*} - U_x^*\partial_{x^*} - U_y^*\partial_{y^*}\right]\tilde{u}_z^* = \hat{\boldsymbol{z}}\cdot\tilde{\boldsymbol{b}}^*, \tag{25a}$$

$$Re_\eta^{-1}\left[\partial_{z^*}^2 + \left(\partial_{z^*}Re_\eta^{-1}\right)\partial_{z^*} - U_x^*\partial_{x^*} - U_y^*\partial_{y^*}\right]\tilde{\omega}_z^* = \hat{\boldsymbol{z}}\cdot\nabla\times\tilde{\boldsymbol{b}}^* + \left(\partial_{z^*}U_y^*\right)\partial_{x^*}\tilde{u}_z^* - \left(\partial_{z^*}U_x^*\right)\partial_{y^*}\tilde{u}_z^*, \tag{25b}$$

Note that, Eq. (25a) is of second order in the vertical direction and of first order in the horizontal directions, hence the Dirichlet boundary conditions which require the perturbed flow

$$\tilde{\boldsymbol{u}}^* = 0, \tag{26}$$

vanishes on the ground, at the city's canopy, on the surface of the buildings, and at the borders of the simulation box cannot be satisfied. To compensate the leading order approximations for the base flow (6) and for the eddy viscosity (11), and to restore the Dirichlet boundary conditions (26), instead of revising boundary conditions as in [3], we propose to replace the analytical inertial term $\boldsymbol{b}^*$ using neural networks. The latter is calibrated from experimental or numerical data to be discussed in the following.

1.3 Poloidal-toroidal decomposition

Instead of the velocity-vorticity formulation, we pursue in this paper the poloidal-toroidal formulation à la Wang et al. [3]. More specifically, the perturbed flow field $\tilde{\boldsymbol{u}}$ satisfying condition (5) can be further decomposed into two scalar potentials [4]

$$\tilde{\boldsymbol{u}}^* = \nabla^*\times\psi^*(x,y,z)\hat{\boldsymbol{z}} + \nabla^*\times\nabla^*\times\phi^*(x,y,z)\hat{\boldsymbol{z}}, \tag{27}$$

where the poloidal $\phi(x,y,z)$ and toroidal $\psi(x,y,z)$ functions are made dimensionless by

$$\phi = \eta UL^2\phi^*, \quad \psi = UL\psi^*. \tag{28}$$

The time averaged velocity field can then be recovered by

$$\overline{u}_x^* = +\partial_{y^*}\psi^* + \partial_{x^*}\partial_{z^*}\phi^* + U_x^*(z), \tag{29a}$$
$$\overline{u}_y^* = -\partial_{x^*}\psi^* + \partial_{y^*}\partial_{z^*}\phi^* + U_y^*(z), \tag{29b}$$
$$\overline{u}_z^* = -\Delta_h^*\phi^*, \tag{29c}$$
$$\overline{\omega}_z^* = -\Delta_h^*\psi^* \tag{29d}$$

where $\Delta_h^* = \partial_{x^*}^2 + \partial_{y^*}^2$ is the two-dimensional Laplacian.

With the decomposition (27), the incompressibility constraint (8) is satisfied by construction. Substituting the relatiosn (29) into Eqs. (15) gives

$$\left[Re_\eta^{-1}\partial_{z^*}^2 + 2(\partial_{z^*}Re_\eta^{-1})\partial_{z^*} - U_x^*\partial_{x^*} - U_{y^*}\partial_{y^*}\right]\Delta_h^*\phi^* = \sigma_\phi^* + e_\phi(x^*, y^*, z^*), \tag{30a}$$
$$\begin{aligned}\left[Re_\eta^{-1}\partial_{z^*}^2 + (\partial_{z^*}Re_\eta^{-1})\partial_{z^*} - U_x^*\partial_{x^*} - U_y^*\partial_{y^*}\right]\Delta_h^*\psi^* &= \sigma_\psi^* + e_\psi(x^*, y^*, z^*) \\ &+ (\partial_{z^*}U_y^*)\partial_{x^*}\Delta_h^*\phi^* - (\partial_{z^*}U_x^*)\partial_{y^*}\Delta_h^*\phi^*.\end{aligned} \tag{30b}$$

where the inertial terms $\boldsymbol{b}^*$ are now replaced by

$$\sigma_\phi^*(x^*, y^*, z^*) = \left[\mathcal{N}_{\sigma_\phi^*}(\boldsymbol{v}^*; \boldsymbol{\theta}_{\sigma_\phi^*})^T \cdot \boldsymbol{v}^*\right], \tag{31a}$$
$$\sigma_\psi^*(x^*, y^*, z^*) = \hat{\boldsymbol{z}} \cdot \nabla \times \left[\mathcal{N}_{\sigma_\psi^*}(\boldsymbol{v}^*; \boldsymbol{\theta}_{\sigma_\psi^*})^T \cdot \boldsymbol{v}^*\right]. \tag{31b}$$

Here, $\mathcal{N}_{\sigma_\phi}(\cdot) : \mathbb{R}^5 \to \mathbb{R}^{5\times 1}$ and $\mathcal{N}_{\sigma_\psi}(\cdot) : \mathbb{R}^5 \to \mathbb{R}^{5\times 2}$ are neural networks, and the input vector consists of 5 mean flow variables

$$\boldsymbol{v}^*(x^*, y^*, z^*) = [u_z^*, \omega_z^*, \partial_{x^*}u_z^*, \partial_{y^*}u_z^*, \partial_{z^*}u_z^*]^T, \tag{32}$$

evaluated locally at each collocation points. Since the calibrated σ_ϕ^* and σ_ψ^* from data are no exact, error terms $e_\phi(x^*, y^*, z^*)$ and $e_\psi(x^*, y^*, z^*)$ are included.

In a domain of size $x \in [-L_x/L, L_x/L]$, $y \in [-L_y/L, L_y/L]$, $z \in [0, L_z/h]$, we consider the following ansatz for the scalar potentials

$$\phi^*(x^*, y^*, z^*) = \sin^2(\pi h z^*/L_z)\,\mathcal{N}_{\phi^*}(x^*, y^*, z^*; \boldsymbol{\theta}_\phi), \tag{33}$$
$$\psi^*(x^*, y^*, z^*) = \sin(\pi h z^*/L_z)\,\mathcal{N}_{\psi^*}(x^*, y^*, z^*; \boldsymbol{\theta}_\psi), \tag{34}$$

such that the perturbed velocity vanishes on the ground and at city's canopy by construction. Here, $\mathcal{N}_\phi(\cdot)$ and $\mathcal{N}_\psi(\cdot)$ are neural networks that map the three-dimensional spatial coordinates to scalars. Solving

$$\nabla^* \times \psi^*(x, y, z)\hat{\boldsymbol{z}} + \nabla^* \times \nabla^* \times \phi^*(x, y, z)\hat{\boldsymbol{z}} = 0, \tag{35}$$

we note that ϕ^* is determined up to a horizontal harmonic function and ψ^* is determined up to an arbitrary function of z. To confine the solution space, we require that

$$\phi^*, \psi^* \geq 0. \tag{36}$$

This is achieved by selecting the output activation of $\mathcal{N}_\phi(\cdot)$ and $\mathcal{N}_\psi(\cdot)$ to be the softplus function.

1.4 Logarithmic velocity profile and linear eddy viscosity

This section explains why there is a correspondence between logarithmic velocity profile and linear eddy viscosity. Denote by u_τ the characteristic shear velocity and the shear stress is given by $\tau = \rho u_\tau^2$. In the logarithmic region, dimension analysis reveals

$$\frac{\partial u}{\partial z} = \frac{u_\tau}{\kappa z}, \tag{37}$$

where κ is a constant. Then the eddy viscosity must depends linearly on z

$$\nu_t \equiv \frac{\tau/\rho}{\partial_z u} = \kappa u_\tau z. \tag{38}$$

2 Numerical observations

2.1 16 Feb

1. $\sigma_\psi = \hat{\boldsymbol{z}} \cdot \nabla \times \mathcal{N}_{\sigma_\psi}$ leads to localised vorticity that extends downstream; whereas $\sigma_\psi = \mathcal{N}_{\sigma_\psi}$ leads to spread vorticity that extends both up- and down-stream.

2. The scale separation between equations for ϕ and ψ leads to spikes in the decay of loss function. Use separate models for σ_ϕ and σ_ψ removes spikes.

2.2 18 Feb.

1. One mode parameterization is efficient, increasing number of modes does not mitigates kinks at edges and corners.

2. The forcing terms σ_ϕ and σ_ψ do vanish on the boundaries.

3. Introducing dependence of σ on $\partial_{x,y,z}\omega_z$ prevents convergence.

2.3 19 Feb.

Tested 4 possible formulations for σ

1. $\sigma_\phi = (\boldsymbol{u} \cdot \nabla)u_z$ and $\sigma_\psi = \hat{\boldsymbol{z}} \cdot \nabla \times (\boldsymbol{u} \cdot \nabla)\boldsymbol{u}$.

2. $\sigma_\phi = (\boldsymbol{u} \cdot \nabla)u_z + \mathcal{N}_{\sigma_\phi}$ and $\sigma_\psi = \hat{\boldsymbol{z}} \cdot \nabla \times (\boldsymbol{u} \cdot \nabla)\boldsymbol{u}$.

3. $\sigma_\phi = (\boldsymbol{u} \cdot \nabla)u_z + \mathcal{N}_{\sigma_\phi}$ and $\sigma_\psi = \hat{\boldsymbol{z}} \cdot \nabla \times (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} + \mathcal{N}_{\sigma_\phi}$.

4. Introducing self-attention mechanism to $\mathcal{N}_\sigma$. Due to limited number of GPUs, I have to stop case study 1 in order to test 4.

5. Observing that the kinks at the edge and corners improves by removing no-slip boundary conditions on the surface of the buildings.

2.4 20 Feb.

1. Introducing analytical part does not improve results.

2. Another place to introduce neural network is at Re_η.

References

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